

X-Ray Spectroscopy and Atomic Data

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ABSTRACT

The Laboratory Astrophysics program employing the Lawrence Livermore National Laboratory (LLNL) Electron Beam Ion Trap (EBIT) has been providing useful atomic data in support of the x-ray missions *Chandra* and *XMM-Newton*. Major achievements have been made for Fe-L ions in hot, collisional plasmas, relevant to stellar coronae, supernova remnants, elliptical galaxies, and galaxy clusters. Measurements for L-shell ions of other cosmically important elements are also required, some of which are in the LLNL EBIT pipeline. On the other hand, data for inner-shell excited lines relevant to photoionized plasmas near accretion sources are largely lacking. Even the wavelengths of these lines are only poorly known, which severely limits their use for diagnostics, despite the great potential.

1. Introduction

With the advent of the high-resolution grating spectrometers on board the *Chandra* and *XMM-Newton* x-ray observatories, spectroscopy has taken central stage in the rejuvenated field of X-Ray Astronomy. The increasing role of spectroscopy as a tool for astrophysical measurements has naturally drawn attention to the relevant atomic physics and atomic data, as those are directly linked with the ability to draw meaningful conclusions from observed spectra. The x-ray wavelength band between 1 and 100 Å, which is covered complementally by the *Chandra* and *XMM-Newton* spectrometers, contains a rich forest of spectral lines emitted by highly charged ions that form at electron temperatures of $kT_e = 0.1 - 3$ keV. At these high temperatures, most of the cosmically abundant elements from C to Ni are stripped down to their K shell (i.e., $n = 1$, n being the principal quantum number) and emit relatively few spectral lines. Additionally, many strong lines of L-shell ($n = 2$) ions of Si to Ni fall in this wavelength range. The eight ionization stages in the L shell can provide more precise information on the temperature structure of the source, independent of elemental abundances, than the two K-shell ionization stages are capable of.

2. The Central Role of Fe-L

The most prominent L-shell x-ray lines in astrophysical spectra are those of iron. Fe-L line emission has been used recently to probe the hot temperature structure in stellar coronal sources (Brinkman et al. 2001), supernova remnants (van der Heyden et al. 2002) and galaxy clusters (Peterson et al. 2001). In general, transitions for both K- and L- shell ions can be calculated with available atomic codes. Nevertheless, in the past, the Fe L-shell lines have been considered highly uncertain, presumably because of the increasing complexity of multi-electron atoms.

To address these issues, an x-ray spectroscopy laboratory-astrophysics program was initiated 11 years ago and is still active today (PI's Kahn and Beiersdorfer). The program is built around the unique capabilities of the LLNL EBIT to measure electron ion interactions. Driven by the astrophysical motivation, these efforts have, so far, focused primarily on the Fe L-shell complex. In particular, high-precision measurements for wavelengths and collisional excitation cross-sections (relative and absolute) have been published. Also, peculiar line ratios of Fe^{16+} that have been puzzling astronomers for years have been investigated and much of the atomic uncertainty has been disentangled from the real astrophysical issues. For more details see the contribution of Brown et al. in these proceedings.

As the first astrophysical grating spectra became available, our team has made a systematic attempt to test the ability of existing models to reproduce the observed emission line intensities. It was found (Behar, Cottam, & Kahn 2001a; Brinkman et al. 2001) that, generally, the observed line intensities could be fairly well reproduced by state-of-the-art distorted wave calculations. For instance, the HULLAC code (Bar-Shalom, Klapisch, & Oreg 2001) was used in those works. In particular, the Fe-L line intensities in the model including all of the high- n lines were found to fare quite well, implying that the calculated excitation rates and ensuing radiative cascades are fairly adequate. Conversely, accurate wavelengths still needed to be incorporated from laboratory measurements. A more detailed confrontation of the atomic calculations with Fe-L spectra of stellar coronae can be found in Behar et al. (2001b), where a comparison of calculations with the spectra of bright stellar coronal sources such as Capella and HR 1099 confirms that, just like the K-shell atomic data, the Fe L-shell data, when calculated correctly, are highly reliable and therefore very useful. The latest versions of the widely used databases MEKAL (Mewe, Kaastra, & Liedahl 1995) and APEC (Smith et al. 2001) now incorporate similar HULLAC data calculated by D. Liedahl with an earlier version of the code.

3. Remaining Atomic Data Issues

Although in general state-of-the-art models are doing well, several discrete, but nonetheless important, discrepancies still remain. In particular, the ratios of the 3s - 2p line intensities relative to those of the 3d - 2p transitions of the same charge state were found to be anomalously high for both Fe^{16+} and Fe^{17+} . Similar effects have also been found in other late-type stars, and even in elliptical galaxies (Xu et al. 2002), which suggests that they are not associated with the astrophysical conditions. The origin of this discrepancy has been recently studied in many theoretical and experimental works (Laming et al. 2001; Doron & Behar 2002; Beiersdorfer et al. 2002), not all in agreement with each other. Additionally, the L-shells of other cosmically abundant elements remain largely unexplored. Major efforts in this direction are being conducted by Lepson et al. (see these proceedings).

This is the place to note that the atomic processes associated with the x-ray emission depend on the type of plasma at the source. So far, we have focused on hot, collisional plasmas that are governed by electron impact ionization and excitation. This type of plasma is relevant to x-ray observations of stellar coronae, supernova remnants, the hot ISM in old galaxies, the intergalactic haloes of galaxy clusters, and to the overwhelming majority of laboratory plasmas. On the other hand, x-ray sources that are ionized and excited by an external radiation field, e.g., active galactic nuclei (AGN) and x-ray binaries, require atomic data for photon impact processes. Modeling line emission from photoionized sources involves radiative recombination and photoexcitation rates (i.e., oscillator strengths). In a recent paper on the x-ray spectrum of the type II AGN NGC 1068 (Kikhabwala et al. 2002), we have shown that the available data for the K-shell ions are very good for reproducing the x-ray spectra from photoionized sources. Work is in progress to test the status of the Fe-L data for photoionized sources. Similar data are routinely used to model absorption spectra. In absorption, however, one also observes inner-shell transitions, for which until recently there was an enormous lack of atomic data.

4. The Urgent Need for Inner-shell Absorption Measurements

The grating spectrometers on board *Chandra* and *XMM-Newton* enable us for the first time to detect x-ray absorption lines due to inner-shell photoexcitation. Since gas under almost any conditions absorbs x-rays, these lines are ubiquitous to x-ray absorption observations. Detections of inner-shell absorption lines have been reported mostly in the ionized outflows of AGN, but also for absorption by neutral ISM. Inner-shell absorption can probe the entire range of ionization states from neutral up to highly-ionized Li-like species. Consequently, these lines impose unprecedented, strict, constraints on the ionization structure

in the absorbing medium. Since there were extremely few relevant atomic data for these features in the literature, in order to analyze the spectra, we had to embark on a tedious endeavor of calculating numerous lines (Behar, Sako, & Kahn 2001c; Behar & Netzer 2002). Calculations by the Ohio State team have also contributed to this effort (Pradhan 2000; Nahar, Pradhan, & Zhang 2001; Pradhan et al. 2002). None of these calculations have been benchmarked in the laboratory.

One case where x-ray absorption lines (including inner-shell excited) are particularly useful is for measuring velocities in AGN outflows (e.g., [kaspi01]). For these measurements, the rest frame wavelengths of the lines need to be known to very high accuracies. The case of inner-shell $K\alpha$ absorption by oxygen is particularly interesting because it could potentially relate the traditional x-ray absorber (O^{6+} and O^{7+}) with absorbers of other wavebands (e.g., O^{5+} in the UV). Whether these absorbers represent the same kinematic systems or not has been debated in the AGN community for some time now. The correct diagnostics of the inner-shell absorption lines could potentially provide a conclusive answer to this interesting astrophysical question. In order to demonstrate the large uncertainties of the currently available atomic data, in Table 1 we present three different calculations for the wavelengths of the strongest $K\alpha$ inner-shell absorption lines of O^{1+} through O^{5+} and also compare them with the deduced wavelengths from the *Chandra*/LETGS observation of NGC 5548, courtesy of J. Kaastra. The wavelengths from NGC 5548 were obtained assuming that the outflow velocities of all ions are similar to that of the well-calibrated O^{6+} velocity. Actually, this assumption may not be valid, but with the lack of laboratory measurements, it provides a rough idea of where to expect these lines.

Although one might have expected the R-matrix method to be the most rigorous, it is clear from the table that at the current state of the atomic data, it is virtually impossible to determine what are the correct rest frame positions of these lines. The discrepancies among the various methods reach 50 mÅ, which corresponds here to uncertainties in the measured velocities of 700 km/s. This uncertainty is of the same order as typical outflow velocities in nearby active galaxies, implying that these lines are practically useless for this purpose, despite their great potential. Laboratory measurements are desperately needed.

5. Suggested Z Pinch Measurements

The currently best available facility for producing inner-shell absorption lines and measuring their wavelengths and optical depths is the z pinch at Sandia National Laboratory. The powerful z pinch experiments (x-ray fluxes reaching 10^{19} erg s $^{-1}$ cm $^{-2}$) produce long-lived (6 ns), steady-state, photoionized gas (Bailey et al. 2001), which can be studied with

high resolution spectrometers, both in emission and in absorption simultaneously. The ionizing spectrum can be characterized rather accurately by a blackbody spectrum. The control over the position and density of the targets in these experiments provides a sensitive handle on the ionization state and column density in the absorbing medium. A demonstration of these capabilities was given by Bailey et al. (2001), where absorption by photoionized Ne has been measured. The spectrum obtained with a crystal spectrometer in that experiment shows many individual lines that are nicely resolved, which allows for accurate wavelength and equivalent-width measurements.

6. Summary and Prospects

Many atomic data needs for hot, collisional plasmas relevant to x-ray spectroscopic observations, now regularly obtained with the gratings on board *Chandra* and *XMM-Newton*, have been provided by the ongoing LLNL EBIT programs of Kahn and Beiersdorfer. Particularly, these programs have provided the most important data for Fe-L emission by hot gas and work is in progress to measure many more high-quality data for other L-shell systems. Now that we actually have high-resolution cosmic spectra, we can determine better than before which atomic data are the most crucial. Thus, the most urgent needs of the x-ray astronomy community for collisional plasmas will continue to be addressed with the EBIT Laboratory Astrophysics Program. Photoionized gases have received less attention as they are more rare in nature and very few laboratory experiments have sufficient x-ray flux to produce them. Particularly missing are measurements for inner-shell absorption lines. The current uncertainties in the positions of these lines considerably limit our ability to use them for diagnostics. In the future, we intend to try to use z pinch experiments to remedy this deficiency.

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Table 1. Wavelengths in Å for the strongest 1s - 2p inner-shell absorption lines in O ions.

Ion	R-matrix ^a	Cowan’s Code ^b	HULLAC ^c	NGC 5548 ^d
O ¹⁺	23.27	23.31	23.30	...
O ²⁺	23.08	23.10	23.11	23.17 ± 0.01
	23.02	23.08	23.05	23.00 ± 0.02
	22.93	23.01	22.98	...
O ³⁺	22.73	22.77	22.73	22.74 ± 0.02
	22.67	22.76	22.78	...
	22.67	22.76	22.73	...
O ⁴⁺	22.35	22.38	22.33	22.38 ± 0.01
O ⁵⁺	22.05	22.05	22.00	22.01 ± 0.01
	21.87	21.85	21.79	...

^aFrom Pradhan et al. (2002)

^bRaassen & Kaastra, private communication

^cPresent work

^dKaastra, private communication